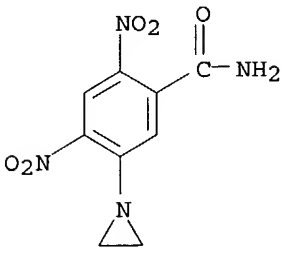
L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 21919-05-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzamide, 5-(1-aziridinyl)-2,4-dinitro- (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2,4-Dinitro-5-ethyleneiminobenzamide
CN 2,4-Dinitroethyleneiminobenzamide
CN 5-(1-Aziridinyl)-2,4-dinitrobenzamide
CN 5-Aziridino-2,4-dinitrobenzamide
CN 5-Aziridinyl-2,4-dinitrobenzamide
CN **CB 1954**
CN NSC 115829
MF C9 H8 N4 O5
LC STN Files: ADISNEWS, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAPLUS, CASREACT, CHEMCATS, CIN, DDFU, DRUGU, EMBASE, IMSDRUGNEWS, IMSRESEARCH, MEDLINE, PROMT, PROUSDDR, RTECS*, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Conference; Dissertation; Journal; Patent
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); PROC (Process); RACT (Reactant or reagent); USES (Uses)
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RLD.NP Roles for non-specific derivatives from non-patents: BIOL (Biological study); PRP (Properties)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C2N	NC2	3	C2N	1.28.1	1
C6	C6	6	C6	46.150.18	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	5.50	pH 1	(1) ACD
Bioconc. Factor (BCF)	5.50	pH 4	(1) ACD
Bioconc. Factor (BCF)	5.50	pH 7	(1) ACD
Bioconc. Factor (BCF)	5.50	pH 8	(1) ACD

Bioconc. Factor (BCF)	5.50	pH 10	(1) ACD
Boiling Point (BP)	427.2+/-45.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	68.22+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	212.2+/-51.7 deg C		(1) ACD
H acceptors (HAC)	9		(1) ACD
H donors (HD)	2		(1) ACD
Koc (KOC)	118	pH 1	(1) ACD
Koc (KOC)	118	pH 4	(1) ACD
Koc (KOC)	118	pH 7	(1) ACD
Koc (KOC)	118	pH 8	(1) ACD
Koc (KOC)	118	pH 10	(1) ACD
logD (LOGD)	1.28	pH 1	(1) ACD
logD (LOGD)	1.28	pH 4	(1) ACD
logD (LOGD)	1.28	pH 7	(1) ACD
logD (LOGD)	1.28	pH 8	(1) ACD
logD (LOGD)	1.28	pH 10	(1) ACD
logP (LOGP)	1.277+/-0.423		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	252.18		(1) ACD
Vapor Pressure (VP)	1.66E-07 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.67 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

153 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
153 REFERENCES IN FILE CAPLUS (1907 TO DATE)

STN.

FILE 'REGISTRY' ENTERED AT 09:28:57 ON 13 JUL 2004
E "5-(AZIRIDIN-1-YL)-2,4-DINITROBENZAMIDE"/CN 25
E "CB1954"/CN 25
E "CB 1954"/CN 25
L1 1 S E3

FILE 'CAPLUS' ENTERED AT 09:31:33 ON 13 JUL 2004
L2 151 S 21919-05-1/RN
L3 3 S L2 AND COSUBSTRATE

FILE 'STNGUIDE' ENTERED AT 09:33:25 ON 13 JUL 2004

FILE 'BIOSIS' ENTERED AT 09:42:13 ON 13 JUL 2004
L4 24 S CB 1954/CN
L5 0 S L4 AND COSUBSTRATE
L6 0 S L4 AND DIHYDROPYRIDINE
L7 0 S L4 AND NAH
L8 0 S L4 AND NRH

FILE 'PCTFULL' ENTERED AT 09:43:44 ON 13 JUL 2004
L9 0 S 21919-05-1/RN
L10 0 S CB 1954/CN
L11 44 S CB1954
L12 3 S L11 AND NRH

WEST Search History

Hide Items | Restore | Clear | Cancel

DATE: Tuesday, July 13, 2004

Hide?	Set Name	Query	Hit Count
	DB=PGPB,USPT,EPAB; PLUR=YES; OP=OR		
☐	L13	L11 and nicotinamide	10
☐	L12	L11 not @py>2000	10
☐	L11	L10 and l7	29
☐	L10	CB adj 1954	37
☐	L9	l7 and L8	5
☐	L8	NQO2	21
☐	L7	prodrugs	19530
☐	L6	l5 and l3	3
☐	L5	bioactivation	310
☐	L4	bioactiviation	1
☐	L3	l1 with (analog or derivative)	778
☐	L2	nicotinamide with analogs	255
☐	L1	nicotinamide	6949

END OF SEARCH HISTORY

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NRH OR "dihydronicotinamide riboside OR Search Advanced Search Preferences

Web Results **11** - **17** of about **21** for **NRH OR "dihydronicotinamide riboside OR "nicotinamide riboside** . (0

Function GO Term Classification
... **dihydronicotinamide riboside** quinone reductase activity; dihydropterin oxidase activity; ... L-ascorbate transporter activity; **nicotinamide** mononucleotide transporter ...
contact14.ics.uci.edu/fgo/function_class_3.html - 33k - Cached - Similar pages

JBC -- Long et al. 277 (48): 46131
... NQO2 uses **dihydronicotinamide riboside** (**NRH**) rather than NAD(P)H as ... **NRH** was synthesized by adding 1,000 units of ... l of 10 mM **nicotinamide** mononucleotide (Sigma ...
www.jbc.org/cgi/content/full/277/48/46131 - Similar pages

[PDF] Disruption of **Dihydronicotinamide Riboside**:Quinone Oxidoreductase ...
File Format: PDF/Adobe Acrobat
... SP4 0JQ, United Kingdom **Dihydronicotinamide riboside** (**NRH**):quinone oxi ... **NRH** was synthesized by adding 1,000 units of ... of 10 m M **nicotinamide** mononucleotide (Sigma ...
www.jbc.org/cgi/reprint/277/48/46131.pdf - Supplemental Result - Similar pages

PNAS -- Zhao et al. 94 (5): 1669
... ionization mass spectrometry; NMNH, reduced **nicotinamide** mononucleotide; QR 1 ... and AK Jaiswal Disruption of **Dihydronicotinamide Riboside**:Quinone Oxidoreductase ...
www.pnas.org/cgi/content/full/94/5/1669 - Similar pages

Bioactivation of 5-(aziridin-1-yl)-2,4-dinitrobenzamide (CB 1954) ...
... NQO2 [NAD(P)H quinone oxidoreductase 2], but its activity is normally latent, and a nonbiogenic co-substrate such as **NRH** [**nicotinamide riboside** (reduced)] is ...
www.ncbi.nlm.nih.gov/entrez/query.fcgi?cmd=Retrieve&db=PubMed&list_uids=10945627&dopt=Citation - Supplemental Result - Similar pages

DISEOME
... M:Receptors, Muscarinic **nicotinamide** histochemistry muscarinic ... derived nondeletion **NRH** detoxified GGGCGGG GSTM1-positive **riboside** gene-environment ...
www.snps3d.org/cgi-bin/tg/ index.pl?key=1728&type=geneShell - 101k - Supplemental Result - Cached - Similar pages

keywords shared by GSTA2 and NQO1 GSTM1 butyl carcinogens oxidant ...
... alleles of the human reduced **nicotinamide** adenine dinucleotide ... H:quinone oxidoreductase 1 (NQO1) and **dihydronicotinamide riboside** (**NRH**):quinone oxidoreductase ...
www.snps3d.org/cgi-bin/tg/edge.pl?n1=2939&n2=1728 - 56k - Supplemental Result - Cached - Similar pages

In order to show you the most relevant results, we have omitted some entries very similar to the 17 already displayed.
If you like, you can repeat the search with the omitted results included.

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NRH OR "dihydronicotinamide rit Search

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